Unstable decay and state selection

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We consider the problem of state selection for a stochastic system, initially in an unstable stationary state, when multiple metastable states compete for occupation. Using path-integral techniques we derive remarkably simple and accurate formulas for state-selection probabilities. The method is sufficiently general that it is applicable to a wide variety of problems.

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The investigation of the decay from a metastable state has been the subject of numerous studies over very many years [1–3]. But the analogous problem of the decay from an unstable state has received comparatively little attention [3–6], and what studies there have been have focussed on the kinetic properties of one-dimensional and quasi-one-dimensional systems [7]. However, these studies cannot address one of the fundamental, open questions in non-equilibrium statistical mechanics: state selection from an unstable state in systems with multiple, isolated minima. Here we present a systematic, intuitive, and analytically tractable method which gives results in excellent agreement with Monte-Carlo simulations.

When driven far from equilibrium many systems encounter instabilities. At such points, noise plays a crucial role. In addition, in complex systems there are multiple modes that interact and can compete. Perhaps the most familiar example is found in Rayleigh-Bénard convection. Consideration of the interaction between two competing modes leads to the following equations for their amplitudes x and y [8]:

$$\begin{aligned}\dot{x} &= \alpha x - \gamma x y^2 - \delta x^3 + \eta_x(t)\\ \dot{y} &= \beta y - \gamma y x^2 - \epsilon y^3 + \eta_y(t),\end{aligned} \tag{1}$$

where α and β are the (positive) growth rates for the two modes x and y, γ is the (positive) coupling coefficient, and δ and ϵ are positive stabilizing coefficients. The variables η_x and η_y are Gaussian random variables with mean zero and variance $\langle \eta_i(t)\eta_j(t')\rangle = 2D\delta_{ij}\delta(t-t')$, where i and j are either x or y, and D is the noise strength. As we are considering the decay from the unstable stationary point $x=0, y=0$, the noise plays an essential role. There are four main elements that are present in Eq. (1): (i) an unstable stationary point with exponential growth of the modes in the neighborhood of this point, (ii) interaction between the modes, (iii) isolated metastable states, and (iv) noise. These features are also found in many other systems [9–11].

In this Letter we address the question: given a system described by equations such as (1), with the initial condition being the unstable stationary point, what is the probability that the system finds itself in a given metastable configuration? The system will relax to thermal equilibrium over a time scale that is on the order of $\exp(E/D)$, where E is a characteristic energy barrier separating the metastable states. However, if $D \ll 1$, this time can be enormous. Our focus is on understanding the occupation over shorter time scales.

Our approach is based on the path-integral representation for the conditional probability density $P(\mathbf{r}, T|\mathbf{0}, 0)$ that the system resides in state $\mathbf{r}$ at time T given that it started at the unstable stationary point at the origin. For purposes of illustration, we take the concrete, physically important example presented in Eq. (1). The path-integral expression for P is given by [12]

$$P = \int \mathcal{D}\mathbf{r}\, J[\mathbf{r}]\, e^{-S[\mathbf{r}]/D} \tag{2}$$

$$\text{where} \quad S[\mathbf{r}] = \frac{1}{4}\int_0^T dt\, [\dot{\mathbf{r}} + \nabla V(\mathbf{r})]^2 \tag{3}$$

$$\text{and} \quad J[\mathrm{r}] = \exp\Big(\frac{1}{2}\int_0^T dt\, \nabla^2 V(\mathbf{r})\Big). \tag{4}$$

Here S is the action, J is the Jacobian, and V is the potential for this problem and is given by

$$V(\mathbf{r}) = -\frac{\alpha}{2}x^2 - \frac{\beta}{2}y^2 + \frac{\gamma}{2}x^2y^2 + \frac{\delta}{4}x^4 + \frac{\epsilon}{4}y^4. \tag{5}$$

To evaluate the path integral for weak noise, a natural approximation scheme is the method of steepest descent. In this approach, the path integral is dominated by the paths of least action; a necessary condition is that these paths make the action stationary. The leading approximation is to simply evaluate the action along these paths. However, in our case it is necessary to go beyond this order and include both (Gaussian) fluctuations about the paths of least action, as well as the Jacobian evaluated along the appropriate path. In other words, once the stationary paths have been determined, we need to calculate three quantities: (i) the action, (ii) the Jacobian, and (iii) the fluctuation determinant, which characterizes the effect of fluctuations about the relevant path.

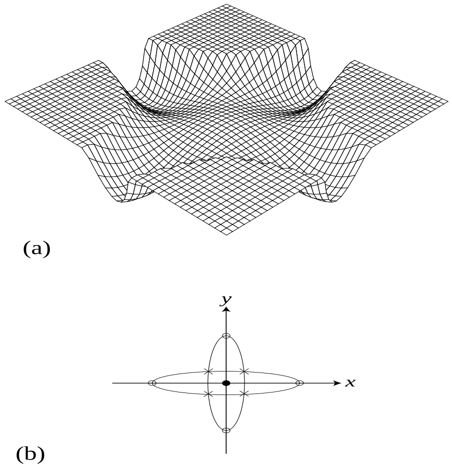

FIG. 1. (a) $V(x,y)$ with $\alpha = \beta = 2$, $\gamma = 4$, $\delta = \epsilon = 1/5$. (b) Contours of zero force.

Having outlined a general prescription for calculating the conditional probability density, we now focus on the specific example introduced above. Figure 1a is a three-dimensional plot of $V(\mathbf{r})$ for a certain choice of parameters. In Fig. 1b we plot the locus of points for which $\nabla V = 0$. This is a useful way to visualize state space; the points where the ellipses intersect each other are the saddle-points of V (denoted by crosses), the points where the ellipses intersect the x and y axes are the local minima (denoted by open circles), and the origin is the unstable stationary point (denoted by a closed circle). The question of interest here can now be phrased in the following way: given an ensemble of systems, each of which starts at the unstable stationary point, what fraction of the ensemble flows into an x-valley or y-valley (which lead to the x- and y-wells, respectively)? For simplicity, we suppose that δ and ϵ are sufficiently small that the local minima are so distant from the region where state selection occurs that they have no influence. Operationally, this consists of setting δ and ϵ to zero, so that now

$$V(x,y) = -\frac{\alpha}{2}x^2 - \frac{\beta}{2}y^2 + \frac{\gamma}{2}x^2y^2. \tag{6}$$

Given that the minima are now irrelevant, it is natural to consider the conditional probability that if the system starts at $\mathbf{r} = \mathbf{0}$ it ends up in an x-valley denoted by $(X,0)$ or a y-valley denoted by $(0,Y)$. To do this we follow the procedure outlined above, viz. we first find the path, or paths, of least action that connect the unstable point to a point in one of these valleys. (Hereafter we shall confine our attention to the calculating the probability that if the system starts at $\mathbf{r} = (0,0)$ at $t = 0$ that it end at $\mathbf{r}_x = (X,0)$ at $t = T$. The analogous problem where the endpoint is $\mathbf{r}_y = (0,Y)$ can be handled in exactly the same way.) The most obvious stationary path is $\mathbf{r}_c = (x_c, 0)$, where

$$x_c(t) = X\frac{\sinh(\alpha t)}{\sinh(\alpha T)}. \tag{7}$$

The action $S_c \equiv S[x_c]$ for this solution is given by

$$S_c = \frac{\alpha X^2}{4}[\coth(\alpha T) - 1] \tag{8}$$

In the limit that $T \to \infty$, $S \to 0$, so that, at least in this limit, this solution is a path of least action, not simply a stationary path. We are unable to prove that this is the only stationary path that connects $(0,0)$ with $(X,0)$. However, we will show that we can make significant progress by considering only this path. In fact, this simplification will enable us to derive a remarkably simple formula for $P(\mathbf{r}_x, T|\mathbf{0}, 0)$.

The second factor that we must evaluate is the Jacobian evaluated along the path $\mathbf{r}_c$. Using Eqs. (4) and (7) we find that

$$J[\mathbf{r}_c] \equiv J_x J_y = \left\{e^{-\frac{1}{2}\int_0^T dt\,\alpha}\right\}\left\{e^{\frac{1}{2}\int_0^T dt\,[-\beta+\gamma x_c^2(t)]}\right\}. \tag{9}$$

It is straightforward to calculate both J_x and J_y, with the results that

$$J_x = \exp\left(-\frac{1}{2}\alpha T\right) \tag{10}$$

and
$$J_y = \exp\left(-\frac{\beta T}{2} + \frac{\gamma X^2}{4\alpha}\frac{\sinh(2\alpha T) - 2\alpha T}{2\sinh^2(\alpha T)}\right). \tag{11}$$

The third quantity that we must calculate is the effect of fluctuations about $\mathbf{r}_c$. To do this, we expand $S[\mathbf{r}]$ about the path $\mathbf{r}_c$, keeping terms of second order. Taking $\mathbf{r} = \mathbf{r}_c + \delta\mathbf{r}$, we have that $S[\mathbf{r}] = S[\mathbf{r}_c] + \frac{1}{2}\int dt\,\delta\mathbf{r}\,L[\mathbf{r}_c]\,\delta\mathbf{r}$, where $L_c \equiv L[\mathbf{r}_c]$ is a 2×2 matrix-differential operator that is given by

$$L[\mathbf{r}_c] \equiv \begin{bmatrix} L_x & 0 \\ 0 & L_y \end{bmatrix} \tag{12}$$

where
$$L_x \equiv -\partial_t^2 + \alpha^2 \tag{13}$$

and
$$L_y \equiv -\partial_t^2 + (-\beta + \gamma x_c^2)^2 - 2(\alpha x_c)(\gamma x_c) \tag{14}$$

The path integral in Eq. (2) over $\mathbf{r}$ now becomes an integral over $\delta\mathbf{r}$. Using the second-order expansion of $S[\mathbf{r}]$, the Gaussian integrals over $\delta\mathbf{r}$ can be completed. These integrals contribute a factor of $\sqrt{|\det L_c|}^{-1}$ to the expression for the conditional probability. As L is block-diagonal, we have that $\det L_c = \det L_x \det L_y$. Combining this with the fact that $J_c = J_x J_y$, the steepest-descent approximation for the conditional probability can be written as

$$P(\mathbf{r}_x,T|\mathbf{0},0) \sim \Omega^{-1}P_0 \tag{15}$$

$$\text{where}\quad P_0 \equiv \frac{J_x}{\sqrt{|\det L_x|}}\mathrm{e}^{-S_c/D} \tag{16}$$

$$\text{and}\quad \Omega^{-1} \equiv \frac{J_y}{\sqrt{|\det L_y|}} \tag{17}$$

The expressions for S_c, J_x and J_y are given in Eqs. (8), (10) and (11), respectively. The conditional probability, P, is the product of two factors: P_0, which is described in the following paragraph, and Ω^{-1}. This form is particularly appealing because, as we shall see below, it is Ω that accounts for the presence of the competing y-mode, whereas P_0 is independent of both β and γ and is therefore insensitive to the presence of y. To determine P_0 and Ω we need to calculate $\det L_x$ and $\det L_y$.

The calculation of $\det L_x$ is straightforward, with the result that $\det L_x \propto \sinh(\alpha T)$. Combining this result with Eq. (8) for S_c and Eq. (10) for J_x, P_0 can be written as

$$P_0(X,T) = \sqrt{\alpha[\coth(\alpha T)-1]}\; e^{\frac{-\alpha X^2}{4D}[\coth(\alpha T)-1]}. \tag{18}$$

P_0 is the conditional probability density that a one-dimensional system under the influence of the potential $-\alpha x^2/2$ and Gaussian white noise be located at $x = X$ at $t = T$ given that it started at $x = 0$ at $t = 0$. As a function of T, P_0 is peaked at a value T^* that is given by $\coth(\alpha T^*) = 1 + 2D/(\alpha X^2)$, i.e.

$$T^* = (2\alpha)^{-1}\ln(1+\alpha X^2/D). \tag{19}$$

The calculation of $\det L_y$ is not as straightforward; it can be expressed as [13]

$$\det L_y = \frac{h_2(T)h_1(0) - h_1(T)h_2(0)}{\dot h_2(0)h_1(0) - \dot h_1(0)h_2(0)}, \tag{20}$$

where h_1 and h_2 are two linearly independent solutions of the homogeneous equation $L_y h = 0$. The denominator of Eq. (20) is the Wronskian of the two solutions. To evaluate Eq. (20), consider the quantity

$$h_1(X,t) = \exp\left(\beta t - \gamma\int_0^t dt'\, x_c(t')^2\right). \tag{21}$$

Taking the second derivative of h_1 with respect to t we find that

$$\ddot h_1 = \Big[(\beta-\gamma x_c^2)^2 - 2(\dot x_c)(\gamma x_c)\Big]h_1. \tag{22}$$

Comparing Eq. (22) with $L_y h = 0$ from Eq. (14), we see that if $\dot x_c = \alpha x_c$ then h_1 is one of the desired solutions. Now $\dot x_c = \alpha x_c\coth(\alpha t)$, so as long as $\coth(\alpha t)$ is close to 1, h_1 is a good solution. Recall, however, that for $T < T^*$, P_0 is essentially zero [c.f. Eq. (18)]. Thus, it is only values of $T > T^*$ that are relevant. But $\coth(\alpha T^*) = 1 + \mathcal{O}(D)$ so indeed we expect that as long as $D \ll 1$, h_1 is a good approximate solution to the homogenous equation $L_y h = 0$. The second linearly independent solution, h_2 can be expressed in terms of h_1 as $h_2(t) = h_1(t)\int_0^t dt'\, h_1^{-2}(t')$. With this choice of h_2, we have that $h_2(0) = 0$. In addition, $h_1(0) = 1$ so that the Wronskian is unity and

$$\det L_y = h_2(T) = h_1(T)\int_0^T dt\, h_1^{-2}(t). \tag{23}$$

Combining this equation with the fact that $J_y = h_1^{-1/2}(T)$ [c.f. Eqs. (11) and (21)], we find that

$$\Omega(X,T) = h_1(X,T)\sqrt{\int_0^T dt\, h_1^{-2}(X,t)}. \tag{24}$$

With this expression for Ω, together with Eq. (21) for $h_1(t)$ and Eq. (18) for P_0, we have succeeded in deriving a formula for $P(\mathbf{r}_x,T|\mathbf{0},0)$ that accounts for the Jacobian prefactor as well as the Gaussian fluctuations about the stationary path $\mathbf{r}_c$. To calculate the analogous formula for $P(\mathbf{r}_y,T|\mathbf{0},0)$ [where $\mathbf{r}_y = (0,Y)$], we simply switch α and β and replace X with Y.

At this stage we are in a position to calculate, using our expression for $P(\mathbf{r}_x,T|\mathbf{0},0)$, the probability that the system flows into a given well. Currently, we have a simple analytic expression for P_0, but to calculate Ω we need to integrate h_1^{-2} over time. This integration presents no difficulty in principle. However, by making two approximations we are able to obtain a simple analytic formula for Ω. Specifically, we approximate the exponential factor $\exp[\frac{\gamma x^2}{\alpha}\frac{\sinh(2\alpha t)}{2\sinh(\alpha T)^2}]$ as $1+\exp[\frac{\gamma x^2}{\alpha}\frac{\sinh(2\alpha T)+2\alpha(t-T)\cosh(2\alpha T)}{2\sinh(\alpha T)^2}]$ and omit the contribution from the lower limit ($T = 0$) in Eq. (23). This second approximation is due to the fact that, as explained in the discussion following Eq. (22), $h_1(t)$ is only a good solution for $\alpha t > 1$. We now obtain the following approximate formula for $\Omega(X,T)$:

$$2\beta\Omega^2 = \exp\left[-\frac{\gamma X^2}{\alpha}\frac{\sinh(2\alpha T)-2\alpha T}{2\sinh^2(\alpha T)}\right]\{\exp(2\beta T)-1\} \tag{25}$$

We have compared Eq. (25) with numerical calculations of Eq. (24), and we find that for the relevant range of parameters the results are essentially indistinguishable. Thus, Eq. (18) for P_0 and Eq. (25) for Ω together provide an analytic formula for the conditional probability given in Eq. (15).

We now turn to the computation of the relative probability that the system flows into an x- or y-valley. The strategy is to calculate the total probability flux through the x-valleys and the y-valleys and compare them. The probability current, which we denote by $\mathcal{J}(\mathbf{r},T)$, is given by $\mathcal{J} = -P\nabla V - D\nabla P$, so that the total flux $\mathcal{F}_x$ through

an x-valley at X is $\mathcal{F}_x(X) = \int_0^\infty dt \int_{-\infty}^{\infty} dy \mathcal{J}_x(\mathbf{r}, t)$ and the total flux $\mathcal{F}_y$ through a y-valley at Y is $\mathcal{F}_y(Y) = \int_0^\infty dt \int_{-\infty}^{\infty} dy \mathcal{J}_y(\mathbf{r}, t)$, where $\mathcal{J}_x$ and $\mathcal{J}_y$ are the x- and y-components of $\mathcal{J}$, respectively. Denoting by N_x the relative probability of flowing into an x-valley we then have that

$$N_x(X, Y) = \frac{\mathcal{F}_x(X)}{\mathcal{F}_x(X) + \mathcal{F}_y(Y)} \tag{26}$$

The calculation of the fluxes requires a knowledge of $\mathcal{J}$ and hence of $P(\mathbf{r}, T|\mathbf{0}, 0)$. In particular, we require this function for an arbitrary point in the x-valley and not just on the x-axis, i.e., we require $P(\mathbf{r})$, not simply $P(\mathbf{r}_x)$. The method we have presented may be extended to obtain the full functional dependence on $\mathbf{r}$ [14], but the results given above do not give P any explicit dependence on the y variable across the x-valley or the x variable across the y-valley. We will therefore limit ourselves here to showing that, by estimating the flux by sampling it on the axis, we can get excellent agreement with Monte-Carlo simulations and therefore confirm the essential correctness of our approach. A feature of this procedure is the necessity of fitting X or Y. We expect that this will no longer be required when the flux is calculated, since this should enable $\mathcal{F}_x(X)$ and $\mathcal{F}_y(Y)$ to be calculated for large X and Y where we would expect them to be insensitive to their actual values. The only restriction that we will impose on X and Y is that they are not too small, for then state-selection will not have occurred when these points are reached. We estimate the minimum value of X to be of the order of X_{min}, the point at which the force in the y-direction changes sign. For V given in Eq. (5) we have that $X_{min} = \sqrt{\beta/\gamma}$. Likewise, we have that the minimum value of y is given by $Y_{min} = \sqrt{\alpha/\gamma}$.

The Monte-Carlo simulations are performed on the Langevin equation with $V(x, y)$ given in Eq. (6). In Fig. 2 the results are shown for a range of values of α and particular choices of β and of γD (γ and D always appear in this combination, since the effect of the interaction is to renormalize the noise). The theory we have outlined here is seen to be in excellent agreement with the simulations. For $\gamma D = 0.1$ we have taken $X = X_{min}$ and $Y = Y_{min}$ and for $\gamma D = 0.001$ we have taken $X = 1.83X_{min}$ and $Y = 1.83Y_{min}$. Comparison for other values of the parameters, a determination of the region of validity of our approximation in parameter space and further improvements of the method will also be discussed elsewhere [14].

In this Letter we have presented a systematic method for determining state selection from an unstable stationary state, when multiple metastable states compete for occupation. Previous methods have not addressed this question directly. Our treatment has the added advantage of yielding closed form, analytic expressions for the conditional probability distribution. Finally, we emphasize that, although we have focussed on a specific potential system with two degrees of freedom for illustrative purposes, our theory is neither restricted to potential problems nor to systems with only two degrees of freedom.

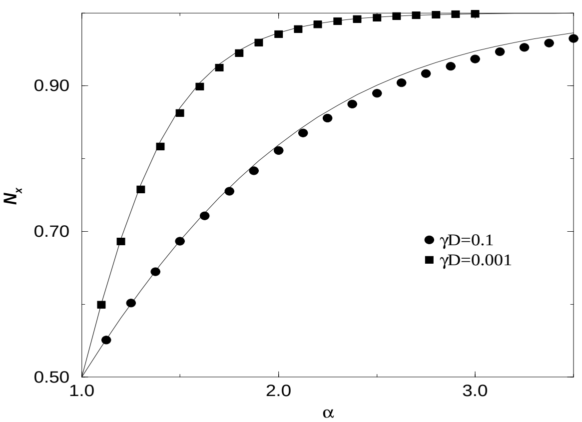

FIG. 2. Probability of flowing into an x-valley as a function of α. Simulation results are for $\beta = 1$ and the continuous curves are our theoretical results.

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